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Research Interests

My field is Computational Materials Science, specifically applications of quantum chemistry and density functional theory for modeling of nanoscale materials. The physical systems I am interested in are diamond surfaces, interfaces, grain boundaries, and the growth processes when diamond films are produced in our laboratories. My current focus is in the integration of various modeling programs, to enable researchers to combine the strengths of each approach to allow solving more complex problems. I also share responsibility for the high-performance computing systems at our center.

Recent Publications

1. A. S. Barnard and M. Sternberg, *Mapping the location and configuration of nitrogen in diamond nanoparticles*, Nanotechnology **18**, 025702 (2007).
2. M. Sternberg, L. A. Curtiss, D. M. Gruen, G. Kedziora, D. A. Horner, P. C. Redfern, and P. Zapol, *Carbon ad-dimer defects in carbon nanotubes*, Phys. Rev. Lett. **96**, 075506 (2006).
3. P. C. Redfern, P. Zapol, M. Sternberg, S. P. Adiga, S. A. Zygmunt, and L. A. Curtiss, *Quantum chemical study of mechanisms for oxidative dehydrogenation of propane on vanadium oxide*, J. Phys. Chem. **110**, 8363 (2006).
4. M. Sternberg, P. Zapol, and L. A. Curtiss, *C₂ adsorption on the (100) diamond surface: Periodic and large cluster calculations*, Mol. Phys. **103** (2005).
5. A. S. Barnard and M. Sternberg, *Substitutional nitrogen in nanodiamond and bucky-diamond particles*, J. Phys. Chem. **109**, 17107 (2005).
6. M. Sternberg, D. A. Horner, P. C. Redfern, P. Zapol, and L. A. Curtiss, *Theoretical studies of CN and C₂ addition to a (100) – (2 Å~ 1) diamond surface: Nanocrystalline diamond growth mechanisms*, J. Comput. Theor. Nanosci. **2**, 207 (2005).
7. M. Sternberg, P. Zapol, and L. A. Curtiss, *Carbon dimers on the diamond (100) surface: Growth and nucleation*, Phys. Rev. B **68**, 205330 (2003).
8. M. Sternberg, M. Kaukonen, R. M. Nieminen, and Th. Frauenheim, *Growth of (110) diamond using pure dicarbon*, Phys. Rev. B **63**, 165414 (2001).